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Work by John D. Joannopoulos and his collaborators is summarized here.

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"Surface and Defect Excitations in Covalently Bonded Solids"

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For Period of February 1, 1986 through January 31, 1990

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Submitted by

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I. PROGRESS

Since the renewal of this proposal on February 1, 1986, we have succeeded in obtaining a fundamental understanding of the electronic structure, magnetic structure, geometric structure, transport properties, and phase transitions and critical phenomena of a variety of systems. Fortunately, we have been extraordinarily productive during this period. The specific systems investigated and some of the results, predictions and implications of our theoretical analyses, are discussed briefly below.

A. DC Conductivity and the Meyer-Neldel Rule in a-Si. Hydrogenated amorphous silicon (a-Si:H) has been intensively studied in recent years. In comparison with crystalline semiconductors, a-Si:H exhibits certain new features. One of these is in the dc conductivity. Unlike crystalline semiconductors, for which the Arrhenius plot is a straight line, n-type doped a-Si:H exhibits a kink at a temperature around 400K.[1] Just below the kink temperature, the Arrhenius plot possesses an unusual concavity. This behavior is illustrated in Fig. 1. While possessing these unique
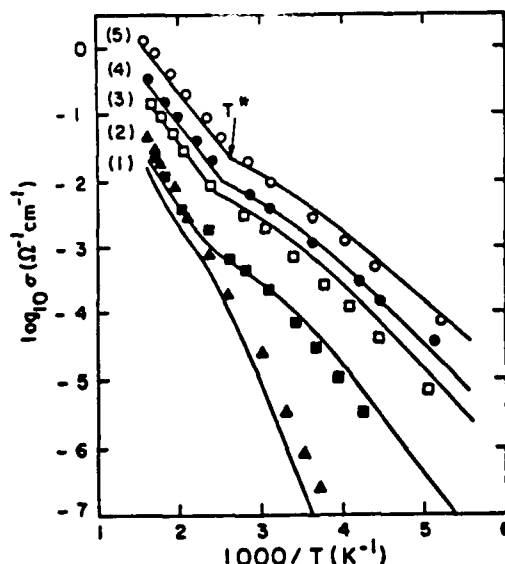

Fig. 1. Comparison of the experimental (Ref. 1) and theoretical Arrhenius plot for various doping levels of phosphorus-doped a-Si:H. (1) 1 ppm, (2) 3 ppm, (3) 250 ppm, (4) 1000 ppm, and (5) 10 000 ppm.

features, a-Si:H exhibits an even more important universal property of the conductivity, known as the Meyer-Neldel Rule.[2] This corresponds to the universal activation energy dependence of the conductivity prefactor and unifies the behavior of different samples prepared under different conditions.

Although a number of theoretical models have been proposed to explain these interesting properties of the conductivity, to date no theory has successfully given a quantitative description which is in agreement with measurements.

Recently, we succeeded by using our general thermodynamic-ensemble theory for disordered systems[3] to model the electronic structure and the extended state conduction model to describe the transport carriers. The central point of the thermodynamic ensemble theory is that the amorphous solid structure itself is determined by the formation free energy of deviations from the effective ground state - an ideally bonded network. This theory assumes that there exists a freezing temperature T*, above which both structural and electronic equilibrium can be reached, but below which the structure is frozen. Applied to a-Si:H, this theory can explain the properties of the band tails, defect states, and the Fermi level dependence on doping and temperature. The results show that the unusual temperature dependence of the Fermi energy completely accounts for the properties of the dc conductivity. In particular, the rapid change in Fermi energy which arises from changes in structural relaxation processes is responsible for the kink that appears in the Arrhenious plot. Morevoer, by investigating the conductivity prefactor under a wide range of conditions (e.g. doping level, transition energy, formation energy, and freezing temperature) we recover the Meyer-Neldel rule. All the theoretical results are in excellent agreement with experiments.

**B.   Ab-Initio   Pseudopotentials   for   Highly
Electronegative 1st Row Elements.** In the last few years
ab-initio pseudopotential density-functional total-energy
calculations have made significant contributions to our
understanding of structural and dynamical properties of
defects, surfaces, interfaces, phase transitions, and
amorphous solids. Highly electronegative first-row atoms
like oxygen and fluorine have, typically, not been studied
because of their compact valence p-orbitals. Such compact
orbitals, which are also involved in bonding, lead to charge
densities which are difficult to represent numerically. While
the compact orbitals suggest a localized basis, plane waves
provide an unbiased basis set for the comparison of different
geometries.   Indeed, experience has demonstrated that
optimization of exponents of localized basis sets for low
symmetry configurations with large atomic displacements is a
very difficult task. We have therefore opted to remain with
plane wave bases.

Pseudopotentials are used extensively in the study of
material properties due to simplifications that enable
realistic calculations while retaining high accuracy.
Pseudopotentials reduce the number of electrons and the
number of basis states required to represent the electrons
relevant for structural properties of materials. Ab-initio
pseudopotentials are constructed to retain specific atomic
valence-electron properties such as eigenvalues and
wavefunctions outside of a small core region. However, the
use of pseudopotentials to soften the electron-nucleus
interaction is much less effective for atoms where core
states do not exist for a particular angular-momentum state -
such as the p orbitals of oxygen and fluorine. The absence
of core states is directly responsible for the existence of
compact nodeless p-orbital wave-functions.

In the usual approach to generating pseudopotentials, and
optimizing the potentials for convergence, one tries to
construct pseudopotentials with rapidly convergent fourier

transform.[4] This, however, does not actually lead to a more rapidly convergent total energy. To accomplish this one needs to focus on the __wavefunction__ and to construct potentials that generate smoother atomic wavefunctions. By modifying the core-size of exisisting pseudopotential techniques[5] we have constructed pseudopotentials with dramatically improved convergence in basis size. The results are shown in Fig. 2 for the case of SiO_2. (Results for
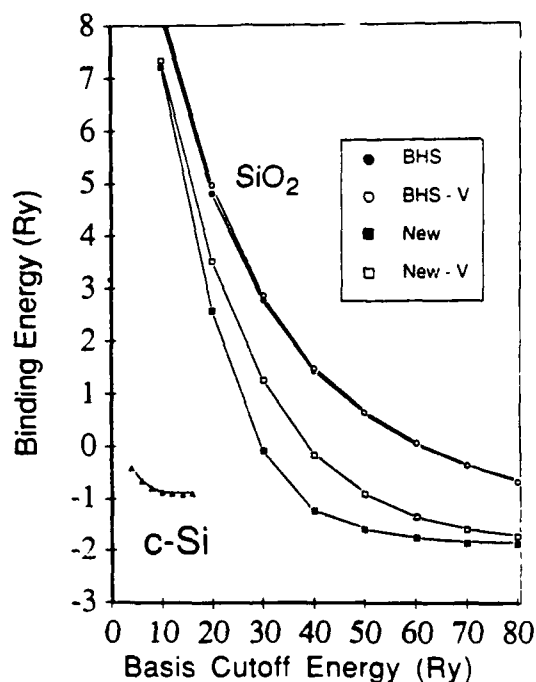

Fig. 2. Convergence of the total Energy with respect to free atoms as a function of the plane-wave basis-set cutoff.

crystalline silicon are also shown for comparison.) The curves marked BHS and BHS-V are for the standard pseudopotential construction[4,5]. The curve marked "New" is designed to give a smoother wavefunction while "New-V" is designed to take "New" and modify it to smooth the potential. It is clear that it is the properties of the atomic wavefunction that are most important in determining the convergence in total energy. This marked improvement in

convergence now makes calculations involving materials with oxygen, and other first-row elements, tractable, for the first time, with ab-initio pseudopotential approaches. This paves the way for future studies of a variety of complex and important material systems.

C. Monte Carlo Study of the Quantum Heisenberg Antiferromagnet. Following the discovery of high-T_c superconductors, great effort has been devoted to understanding their magnetic properties. This has been motivated by the possibility of an intimate connection between magnetic behavior and the mechanism for the new superconductivity.[6] Neutron scattering experiments[7] on the prototype La_2CuO_4 have indeed revealed a rich magnetic structure. In particular, over a substantial range of temperatures, very strong antiferromagnetic correlations in the Cu-O planes have been observed with large correlation lengths but no long range order. These features are modelled well by a quantum spin-1/2 Heisenberg antiferromagnet on a planar square lattice.

Aside from its significance for high T_c-Superconductivity, the spin-1/2 Heisenberg antiferromagnet is an interesting theoretical model in its own right. Quantum fluctuations are believed to play an important role but it is not clear how they might affect the behavior one would expect from the classical model. Even the existence of order in the ground-state has been controversial.[8]

In order to investigate the equilibrium properties of this quantum system, we used the Monte Carlo scheme developed earlier[9] for antiferromagnets, and introduced a new sampling procedure that dramatically improves the exploration of configuration space. With this approach it was possible to calculate the energy, specific heat, uniform and staggered susceptibilities, and correlation functions as a function of temperature for lattices of up to 256 spins. The correlation length as a function of temperature was then deduced from the

correlation functions and found to be consistent with a quantum renormalized classical approximation. Using a finite-size scaling analysis we were able to show that the correlation length is inconsistent with a topological-defect-driven phase transition as suggested by others.[10] Moreover, with no adjustable parameters, excellent agreement is obtained betwen the calculated and experimental correlation lengths in La_2CuO_4. Finally, our predictions for the uniform susceptibility appear to have been confirmed by very recent experimental measurements.[11]

D. Magnetic Properties of the Bose Gas. Since the fifties, it has been known that a charged condensed Bose gas in $d > 2$ dimensions exhibits the Meissner effect.[12] These observations led to the concept of the SBB superconductor[13] where resonant two-electron states, bound in position space, form in a solid providing a charged Bose gas that, when condensed, gives rise to superconductivity as evidenced by the Meissner effect. Calculations predating the discovery of the new high-T_c supercondctors suggested that such SBB superconductors might be realizable in nature and have high transition temperatures.[14] Thus the magnetic behavior of the Bose gas is germane to a potential model for high-T_c superconductivity, as well as of interest as an excactly soluble theoretical model exhibiting superconducting and unusual thermodynamic behavior.

To investigate this system we calculate a variety of thermodynamic functions in the presence of a uniform magnetic field and thereby deduced the H-T phase diagram. Contrary to previous theoretical investigations, we find a line of first-order transitions rather than second-order. Though small, they make the Bose gas act like the familiar superconductors more than previously thought. Except for temperatures well within a percent of T_c, the discontinuity in B versus H is independent of particle density and proportion1 to T^2. We find that the first-order nature of the transitions is due to

a novel entropy effect related to the B-dependent Landau degeneracy. We have termed this transition "entropy-driven." The line of first-order transitions terminates in critical points both at T_c and at $T = 0$! The entropy-driven nature of the first-order transitions explains how the low temperature side of the line can terminate in a critical point.

To investigate the effects of a spacially varying magnetic field, a Landau-Ginzburg theory was constructed. The results show that the Bose gas is always a type I superconductor; thus there is no vortex state and the sharp transitions remain. Finally, we note that the new high-T_c superconductors appear to be intrinsically type II. Thus, this work sheds doubt on the hypothesis that they can be understood as SBB superconductors.

E. Symmetry Breaking and Quantum Molecular Dynamics. During the past several years a promising new approach has emerged for performing quantum molecular dynamics simulations. It is based on a scheme first introduced by Car and Parrinello.[15]

The scheme created a great deal of excitement because it promised to achieve global minimization of the total energy of a solid with respect to both electronic and ionic coordinates. Thus implying that structural determination in solids could now proceed essentially by simulated annealing.

Although this approach seemed very promising at first, it turned out to be extremely time consuming in practice. The essential difficulty was the following. In these calculations the electronic system must be close enough to the groundstate of the ionic configuration for the forces to give the correct direction of ionic motion in which the total energy of the system is reduced. Therefore, the rate of relaxation of the electronic system to its zero-kinetic-energy state determines the maximum speed at which the ionic configuration can change and, hence, the number of timesteps required to achieve global energy minimization. This number turned out to be

significantly large to prohibit studies of complex and interesting physical systems.

Three years ago, however, we made a significant modification to the Car and Parrinello approach that made realistic molecular dynamics simulations tractable. Very briefly, our method involves renormalizing away the very rapid oscillations of the electron system which then significantly increases the rate of electronic relaxation. The improvement is striking as shown in Fig. 3. The results are for a model system of an eight atom unit cell of germanium with 4096 plane waves. We can obtain convergence in 1/10 the number of time steps.
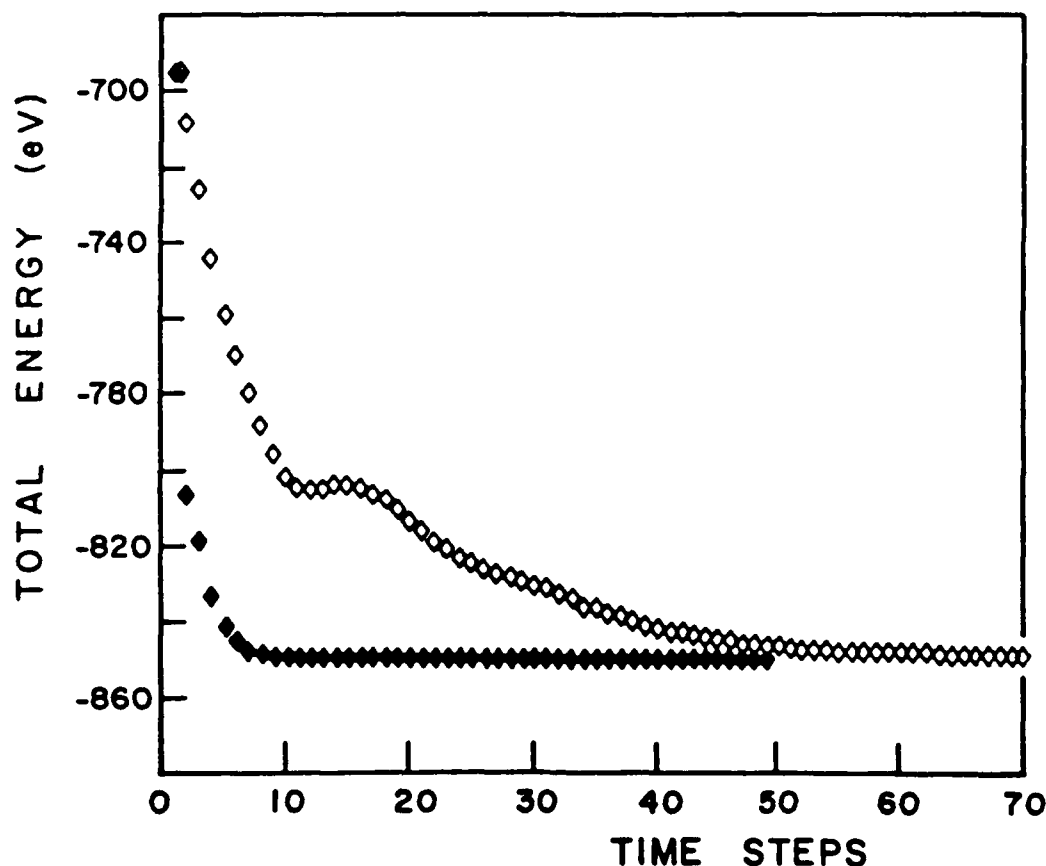

Fig. 3. Convergence tests for Car-Parrinello (open diamonds) and renormalized method (filled diamonds).

But even with this innovation, the original molecular dynamics approach[15] contained a severe flaw. By performing a careful and detailed analysis of the symmetry of the electron wavefunctions as they evolve under the EOM, we found that certain spurious symmetries in the initial conditions (i.e. two or more bands being "partner functions") could prevent wavefunctions from converging to eigenfunctions of the Hamiltonian. This is because the artifical symmetries were conserved throughout the EOM and the original Lowdin orthogonalization procedure. In contrast, we found that using a Gram-Schmidt orthogonalization scheme breaks this symmetry so that the states are always allowed to reach eigenstates. Furthermore, this natural symmetry breaking is desirable for the atomic relaxations as well. This is because it allows the atomic system to explore regions of phase space which have lower symmetry than the original configuration! Finally, the Gram-Schmidt scheme is preferable when one wants to compute the energies of metallic materials, or semiconductor defects with partially filled bands. In the original approach[15] one would have to perform partial diagonalizations of the Hamiltonian at each time step.

F.   Antisites,   Bond-Switching   Reactions   and Negative-U Defects in Chalcogenides. The chalcogenide materials are semiconducting solids that differ from the simpler, tetrahedrally bonded, zincblende compounds in two important respects. Firstly, the molecular nature of the solids, in combination with the low average coordination number, gives rise to very flexible structures. Secondly, the top of the valence band consists of nonboding lone-pair orbitals that are prone to forming bonds with any available atoms. This flexibility of structure and inherent reactiveness of nonbonding orbitals lowers the formation energy of point defects in the chalcogenides and introduces strong coupling between the electronic states of the defects and their geometric structure. Many different types of

defects have been proposed to exist in large concentrations in these materials[17], but all these suggestions have been limited to speculation. The difficulties lie in that the structural complexity of these materials does not allow simple and straightforward interpretation of experimental data in terms of specific defects and has not permitted theoretical arguments based on realistic ab-initio calculations.

The new developments in quantum molecular dynamics simulations (described in section I.E.) provide precisely the calculational capability and predictive power necessary to address these issues in a realistic fashion.

Using As_2Se_3 as a prototype, we performed a systematic and exhaustive study of the lowest energy simple point defects. In this material, these defects are typically antisites and antistructures that conserve the number of bonds. We analyzed twelve different defects and calculated their formation energies, concentrations, and their electronic gap states energies and localization. Two very interesting and important results emerged from this study.

Firstly, we discovered a new and special class of low energy defects. These defects originate from certain antistructures which can undergo a bond-switching transformation leading to the formation of "bond-switched antistructure defects." These are very low energy defects that should be prevalent in the chalcogenide material. They lack deep-gap states and they are probably unique to the chalcogenide materials. One of these "bond-switched antistructure defects" is of particular interest in that it forms a cross-linking bond between the layers of As_2Se_3! Morevoer, it is found that the associated bond-switching reaction proceeds with small or no barrier for most charge states.

Finally, we found one, and only one, defect that had a negative effective correlation energy! The existence of such a defect had been predicted theoretically in 1975 in order to

account for some ve_; :r.usual experimental observations.[18] It has take: 13 years to identify the defect. In particular, we find th t two noninteracting neutral Se antisite defects are unstable toward the formation of a pair of noninteracting oppositely charged Se antisites. The charged antisites are one-fold and three-fold coordinated respectively and provide a gain in correlation energy of 0.3 eV per electron pair.

The results of this project are a sparkling example of the power and usefulness of ab-initio total energy calculations.

II. PUBLICATIONS AND PRESENTATIONS UNDER THIS PROJECT

A. Publications in Referred Journals

1. D.H. Lee, J.D. Joannopoulos, J.W. Negele and D.P. Landau, "A Symmetry Analysis and Monte Carlo Study of the Frustrated Anti-ferromagnetic Planar (XY) Model in 2D," Phys. Rev. B33, 450 (1986).

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